Solvent Influence on the Absorption Spectra of Hydrogen Bonded Complexes

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IR absorption spectra of hydrogen bonded complexes Xe…HF, $(CH_3)_2O$…HF and CF_3CH_2OH…$O(CH_3)_2$ in the region 4300-2500 cm^{-1} were studied. Main conformities of the surroundings influence on valent vibration ν_{AH} absorption band shape at the transition from gas phase to solution and at different solvents was analysed.

It was shown, that at the transition from gas to liquid with an increase of the system density the complexes band is gradually symmetrised and is shifted toward to low frequencies. Since complexes bands have a complicated shape, therefore as characteristic of bands were used the normalized spectral moments which were calculated from experimental spectra.

For complex Xe…HF at small densities of Xe the band has the asymmetric shape. With density increasing at first disappears the band structure and band is shifted forward to low frequencies. At the further increasing of density the band is symmetrised. In liquid Xe is observed enough wide and practically symmetric band of Xe…HF complex. The low-frequency shift of band and the increasing its effective halfwidth define the values of first and second spectral moments of band

ρ (Xe) = 10 Amaga	$M_1=\nu_1$=3951 cm^{-1}	$2\sqrt{M_2}$ =30 (5) cm^{-1}
120	3938	30
280	3923	42
400	3900	47

For CF_3CH_2OH…$O(CH_3)_2$ complex, where $\Delta H \approx 6$ kcal/mol, the influence of solvent is displayed first of all in the increasing of low-frequency shifting of bands as compared with gas phase.

	Gas(T=299 K)	Xe(234K)	Freon-114 B_2 (192 K)
$M_1=\nu_1$, cm^{-1}	3477	3445	3352
$2\sqrt{M_2}$, cm^{-1}	113	92	140

The halfwidth of the band is narrowed as temperature decreases and is broadened as the solvent activity increases.

In mixture $(CH_3)_2O$…HF_+Xe as the Xe density increases the gravity center of complicated band ν_{HF} is shifted forward to low-frequencies

ρ (Xe), Amaga	12	102	294
$M_1=\nu_1$, cm^{-1}	3484	3460	3430

The hydrogen bonded complexes band ν_{AH} at transition from gas to liquid phase is symmetrized and shifted forward to low-frequencies in all studied cases.